Combined continuum and molecular methodology for micro- and nano- scale flows through filters

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The goal of the study is to develop a combined continuum and molecular methodology to compute micro- and nano- scale flows for which slip boundary conditions are important. A novel hybrid method combining the boundary singularity method (BSM) for solving Stokes equations for the entire domain and the direct simulation Monte Carlo (DSMC) for area near rigid boundaries is proposed, tested and implemented. Multi-processor parallel computer algorithm is developed and implemented; however, there is significant future research in more fine-grain parallelization with large amount of processors involved.

For micro- and nano- fluidic systems the Reynolds number $Re<1$ and the ratio of molecular mean free path to characteristic geometric length, the Knudsen number, $Kn>0$. When $Re<1$ non-linear Navier-Stokes equations are replaced with linear Stokes equations. The boundary singularity methods (BSM) are advantageous compare to traditional finite-volume methods for micro-fluidic systems described by Stokes equations because they eliminate the need to mesh 3-D micro-fluidic set-up, which may be geometrically complex and unsteady. For example, dynamics of particles and fluids in micro- and nano- fibrous filters and membranes involve motion of fibers assembled in irregular network. The presence of dynamically adjusting nano- fibers would require dynamic 3-D re-meshing if traditional finite-volume methods are used. On the contrary, using BSM only surface of fibers need to be meshed with observation points, in which boundary conditions need to be satisfied. Modeling of flowfield to predict particles' dynamics in fibrous structures is of significant interest. While cell models for predicting the filter capturing efficiency and pressure drop of fibrous media are available, more detailed models of flowfield are currently needed for sensing and signaling purposes, for example, to predict the position of the adsorbed particles including viruses within the multi-modal non-structured fiber web.

Gas flows around nano-scale fibers and particles [2] typically are in transitional molecular-to-continuum regime ($Kn\sim1$) and, therefore, traditional no-slip boundary conditions are no longer valid while heuristic partial slip conditions are verified for $Kn\leq0.1$ and need to be used with caution for higher Kn. Thus first-principles based molecular methods are needed to adequately model the near-wall layer of flow. On the other hand, molecular methods are still too computationally expensive to use them for entire domain. Therefore combined continuous BSM and molecular methods could be a feasible approach.

A novel hybrid method combining the continuum approach based boundary singularity method (BSM) for the entire domain and the molecular direct simulation Monte Carlo (DSMC) method for near rigid boundary sub-domain has been developed in this study and then used to model viscous fibrous filtration gas flows in the transitional flow regime ($Kn\leq1$).

The DSMC procedure is computationally expensive. The schematic of the parallelization is presented in Figure 1. The BSM with optimized location of singularities is made fairly efficient by the previous research of the authors [3,4,5] so it was performed in a single processor. After the BSM procedure is completed, at a coupling iteration, the boundary conditions for the DSMC procedure are passed to a number of processors, which carry out the DSMC calculations, and vice-versa. If the number of processors equals the number of fibers, DSMC computations corresponding to area surrounding single fiber will be carried by a single processor.

The algorithm was tested first for a flow about single fiber surrounded by cylindrical enclosure. The computational parameters of the coupled BSM-DSMC algorithm are chosen as follows: the thickness of the DSMC area is 3λ; the number density of simulated particles, $\rho_p = 3000$, which corresponds to 7.5 simulated particles in a cell with a size of 0.5λ. It is observed that the DSMC procedure converges steadily with respect to the number of sampling. The proposed hybrid BSM and DSMC method converges with the number of couplings between DSMC and BSM albeit slight variations are still visible after three couplings. For *Kn=0.1*, the results obtained by DSMC, BSM, and coupled BSM-DSMC coincide well. Next, for *Kn=0.5* and *Kn=1* significant difference in profile of slip velocity is observed for results obtained by (i) BSM with heuristic partial slip boundary conditions and (ii) combined BSM and DSMC.

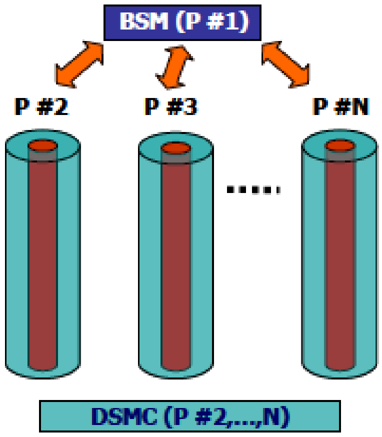

Figure 1: Schematic of parallelization of coupled BSM and DSMC algorithm

Computational results for set of fibers with the same set-up as experiments [9] are obtained using parallel algorithm for combined BSM-DSMC. Results are compared to the BSM method with heuristic partial slip boundary conditions. While results for *Kn<0.1* are very similar for both methods, they differ significantly for *Kn=0.5* and *Kn=1* that confirms the need for combined BSM-DSMC.

Conclusions. Combined continuum and molecular method was proposed to solve micro- and nano- fluidic problems. The method combines boundary singularity method (BSM) for continuum Stokes equations and Direct Simulation Monte Carlo (DSMC) method for near-boundary gas flows for *0.1<Kn<1*. The DSMC allows for precise prediction of slip velocity. Comparison of BSM with heuristic slip boundary condition to combined BSM-DSMC approach shows significant difference in values of slip velocity for isolated fiber and in pressure drop through the set of fibers. The parameters of coupled algorithm were obtained such as thickness of DSMC zone, size of DSMC cell, density of representative particles, and number of coupling iterations between DSMC and BSM. However, the accuracy of coupled BSM-DSMC comes with significant computational overhead compare to heuristic partial slip boundary conditions. Thus parallelization of coupled method is needed and it was implemented and tested in two multi-processor computers. Parallelization efficacy and details of concurrency and data motion will be discussed in our presentation.

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